

3H-1,2-Dithiole-3-thione, 4-methyl-
3354-41-4 | DTXSID30187196

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 253 °C

Global applicability domain: Inside

Local applicability domain index: 3.94e-01

Confidence level: 4.92e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Dithiolane-2-thione

Measured: 307

Predicted: 284

Image not found

Benzenethiol, 4-bromo-

Measured: 231

Predicted: 222

Image not found

Benzene, 1-chloro-4-iodo-

Measured: 227

Predicted: 226

Image not found

Benzene, 1-bromo-4-iodo-

Measured: 252

Predicted: 259

Image not found

1,4-Dibromobenzene

Measured: 219

Predicted: 224